This question paper contains 4 printed pages

M.Tech. / II Sem.   J

NANOSCIENCE AND NANOTECHNOLOGY

PAPER NSNT-202   Computational Methods

Time   3 hours   *Maximum Marks*   38

Attempt any four questions
All questions carry equal marks

1 (*a*)   Explain Newton-Raphson method of finding a
root of the equation $f(x)=0$ Show that it has a
second order convergence Use the method to
find root of the equation $x \sin x - 1 \cdot 0 = 0$, starting
with $x = 1 \cdot 0$ and use three iterations only $5_{1/2}$

   (*b*)   Explain Ramanujan's iterative method which can
be used to determine the smallest root of the
equation $f(x)=0$. Use this method to find the
smallest root of $x^3 - 6x^2 + 11x - 6 = 0$ 4

2 (*a*)   Establish Newton's forward difference inter-
polation formula and the remainder terms (error
in   the   formula)   in   terms   of   appropriate
derivatives Find the value of $e^{1\,17}$ using Gauss

P T O

forward formula from the following data (for x and e^x): (1 . 2 7183), (1 05   2 8577); (1 10   3 0042), (1 15   3 1582), (1 20   3 3201), (1 25   3 4903) and (1 30   3 6693) $5_{1/2}$

(b)   Define the operators $\Delta, \nabla, \delta, E$ and μ and show:

(ı) $\mu E = E\mu$

(ıı) $\mu^2 = 1 + \frac{1}{4}\delta^2$

                                                                                     4

3 (a)   Use Gauss Quadrature method based on intervals of unequal width to calculate a definite integral Calculate the weights and abscissae for $n=2$. Obtain the first four Legendre polynomials using recurrence relation

$$(n+1)P_{n+1}(u) = (2n+1)uP_n(u) - nP_{n-1}(u).$$

Take $P_0(u)=1$ and $P_1(u)=u$ 6

(b)   Use four point Gauss-Legendre formula to evaluate the integral $\displaystyle\int_0^{1/2} \frac{1}{\sqrt{1-x^2}}\, dx$

Abscissae and weights are

$\pm u_ı = 0 \cdot 33998$ $w_ı = 0 \cdot 65215$

$\pm u_ı = 0\ 86114$ $w_ı = 0 \cdot 34785$ $3_{1/2}$

4 (a) Discuss the finite difference method in a two point linear boundary value problem in an ordinary differential equation and estimate the error involved in this method

Use second order Runge-Kutta formula to evaluate $\frac{dy}{dx} = x+y$; where $y(0)=1$; for $x=0\cdot3$, take $h=0\cdot1$ $5_{1/2}$

(b) Describe with equation Adams-Moulton method (Predictor-Corrector formula) to find the solution of a differential equation   4

5 (a) Obtain the expressions for the best value of the slope and intercept and their standard errors using least square method $5_{1/2}$
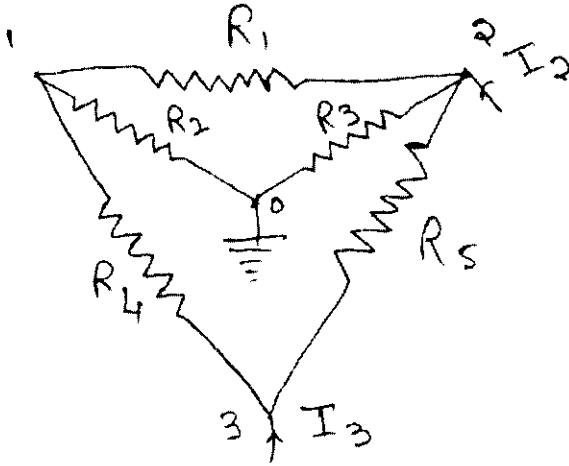
(b) Discuss different types of errors in an experimental data, standard error in a single and a set of observations   4

6 Attempt any *two* of the following $9_{1/2}$

(i) Obtain Trapezoidal formula for the evaluation of a definite integral Work out the error involved in this method

(ii) Obtain the electron-density equation for a crystal in terms of scattering amplitude and location of the atoms in a crystal using Fourier transforms

(iii) Write the admittance and current matrix of the following circuit and find the voltage vector using matrix operations

$$R_1 = R_2 = R_3 = 1\,\Omega$$

$$R_4 = R_5 = 2\,\Omega$$

$$I_2 = 1\ \text{amp}$$

$$I_3 = 2\ \text{amp}$$